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AUG 79 S CHAKRAVARTY, M B FOGEL, W KOHN N00014-76-C-0050

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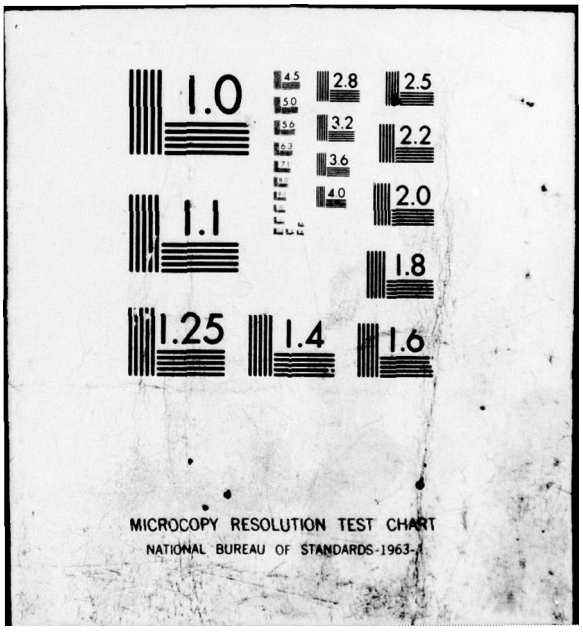
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This paper presents a theory of the linear density response to an external time dependent scalar potential for a Fermi system whose unperturbed density varies slowly on a scale $\ell >> p_F^{-1}$, where p_F is a characteristic Fermi momentum. Simple local density functional response theory is valid except in a region of small q and ω (wave number and frequency of the perturbation). For this region we have worked out a generalization, to the case of inhomogeneous systems, of the classical Landau Fermi liquid theory.

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Dynamic Response of Inhomogeneous Fermi Systems

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ABSTRACT

This paper presents a theory of the linear density response to an external time dependent scalar potential for a Fermi system whose unperturbed density varies slowly on a scale $\ell \gg p_F^{-1}$, where p_F is a characteristic Fermi momentum. Simple local density functional response theory is valid except in a region of small q and ω (wave number and frequency of the perturbation). For this region we have worked out a generalization, to the case of inhomogeneous systems, of the classical Landau Fermi liquid theory.

This paper deals with Fermi systems at zero temperature whose unperturbed density, $n_o(\underset{\sim}{r})$, varies slowly on a scale $\ell >> p_F^{-1}$, where p_F is a typical local Fermi momentum. We wish to calculate the linear density response of such a system to an external scalar potential, $v_1^e(\underset{\sim}{r},t)$, which we write as

$$v_1^e(\underset{\sim}{r},t) = \frac{1}{(2\pi)^4} \int v_1^e(\underset{\sim}{q},\omega) e^{i(\underset{\sim}{q}\cdot\underset{\sim}{r} - \omega t)} d\underset{\sim}{q}\, d\omega \qquad (1)$$

For the time being we consider only neutral systems with short range forces; extension to charged systems poses no significant problems.

For several (overlapping) regimes of q and ω the necessary theory is already available. In view of the slow spatial variation of $n_o(\underset{\sim}{r})$, a plausible ansatz for the density response is the local density approximation

$$n_1(\underset{\sim}{r},\omega) = \int \chi\,(\underset{\sim}{r}-\underset{\sim}{r}',\ \omega;\ n_o(\underset{\sim}{r}))\ v_1^e(\underset{\sim}{r}',\ \omega)\ d\underset{\sim}{r}' \ , \qquad (2)$$

where $\chi(\underset{\sim}{r}-\underset{\sim}{r}',\ \omega;\ n_o)$ is the dynamic response function of a system of uniform density, n_o. This ansatz is in fact valid under the following circumstances:

(I) $\omega << v_F q$ (v_F = Fermi velocity). In this case χ is to a good approximation the static χ, which is known to have a short range of the order of p_F^{-1} or of the range of the forces (region (I) in Fig. 1).

(II) $\omega >> v_F/\ell$. Again χ has a short range of the order of v_F/ω or p_F^{-1} (region (II) in Fig. 1).

(III) $q >> \ell^{-1}$. Here q denotes a characteristic wave-number of V_1^e. The effective range of χ is no larger than q^{-1} (region (III) in Fig. 1)[1].

It can be seen from Fig. 1, that there is a region, R, shown enclosed by heavy lines, which is not covered by the above three regions. Here we develop a theory which is valid in the following regime, (IV) $q \ll p_F$, $\omega \ll p_F^2$ (region (IV) in Fig. 1, shown enclosed by dashed lines). This is the region of validity of the classical Landau theory of Fermi liquids.[2] If ℓ is large enough, region (IV) includes R, and therefore our theory compliments the local density approximation (2).

Our theory is the generalization of Landau theory for systems of slowly varying density. Since the Landau theory for homogeneous systems is valid for long wavelength perturbation, it is plausible that it can be extended to inhomogeneous systems whose unperturbed density varies on a scale ℓ large compared to p_F^{-1}.

For a homogeneous system, subject to an external potential $v_1^e(\underset{\sim}{r},t)$, the Landau transport equation for the quasiparticle distribution function, $n_1(\underset{\sim}{p},\underset{\sim}{r},t)$, is obtained from the classical Hamilton's equations using the effective Hamiltonian

$$H(\underset{\sim}{p},\underset{\sim}{r},t) = \varepsilon(\underset{\sim}{p}) + v_1^e(\underset{\sim}{r},t) + \sum_{\underset{\sim}{p}'} f_{\underset{\sim}{p}\underset{\sim}{p}'}\, n_1(\underset{\sim}{p}',\underset{\sim}{r},t) \ . \tag{3}$$

Spin indices have been suppressed. Here

$$\varepsilon(\underset{\sim}{p}) = \frac{p^2}{2m^*} - \frac{p_F^2}{2m^*} \tag{4}$$

is the one particle energy and the last term arises from short range quasi-particle interactions. Our generalization for an inhomogeneous

system is

$$H(\underset{\sim}{p},\underset{\sim}{r},t) = \varepsilon(\underset{\sim}{p},\underset{\sim}{r}) + v_1^e(\underset{\sim}{r},t) + \sum_{\underset{\sim}{p}'} f_{\underset{\sim}{p}\underset{\sim}{p}'}(\underset{\sim}{r})\, n_1(\underset{\sim}{p}',\underset{\sim}{r},t) \qquad (5)$$

where

$$\varepsilon(\underset{\sim}{p},\underset{\sim}{r}) \quad \frac{p^2}{2m^*(\underset{\sim}{r})} - \frac{p_F^2(\underset{\sim}{r})}{2m^*(\underset{\sim}{r})} \quad ; \qquad (6)$$

$f_{\underset{\sim}{p}\underset{\sim}{p}'}(\underset{\sim}{r})$, $m^*(\underset{\sim}{r})$ and $p_F(\underset{\sim}{r})$ are equal to the homogeneous Fermi liquid parameters $f_{\underset{\sim}{p}\underset{\sim}{p}'}$, m^* and p_F evaluated for the local density, $n_o(\underset{\sim}{r})$. This ansatz is in the spirit of local density functional theory[3] where all local physical quantities are determined by the local density.

The single particle energy $\varepsilon(\underset{\sim}{p},\underset{\sim}{r})$ can be derived from the theory of single particle properties of the inhomogeneous electron gas[4]. It can also be understood as follows. The local wave number of a quasiparticle of vanishing excitation energy is equal to

$$p_F(\underset{\sim}{r}) = \left[3\pi^2 n_o(\underset{\sim}{r})\right]^{1/3} . \qquad (7)$$

(This relationship is unaffected by interactions). In a system in equilibrium, quasiparticles of vanishing excitation energy must have the same single particle energy at any two points $\underset{\sim}{r}_1$ and $\underset{\sim}{r}_2$. In view of (7) this is correctly described by the expression (6). Further, at a given $\underset{\sim}{r}$, the momentum dependence of ε for small $p - p_F(\underset{\sim}{r})$ must be given by the local value of $m^*(\underset{\sim}{r})$ as is the case for our expression (6).

The external perturbation, v_1^e and the interaction term of H are the same as in the homogeneous Landau theory, except that,

because of the short range of the interaction, $f_{\underset{\sim}{p}\underset{\sim}{p}'}(\underset{\sim}{r})$, is not a constant but corresponds to the local density.

The collisionless transport equation is

$$\frac{\partial n}{\partial t} + \underset{\sim}{p} \cdot \nabla_{\underset{\sim}{p}} n + \underset{\sim}{r} \cdot \nabla_{\underset{\sim}{r}} n = 0 \tag{8}$$

where $\underset{\sim}{p}$ and $\underset{\sim}{r}$ are determined by Hamilton's equations,

$$\underset{\sim}{p} = - \nabla_{\underset{\sim}{r}} H \; ; \; \underset{\sim}{r} = \nabla_{\underset{\sim}{p}} H \tag{9}$$

We write

$$n(\underset{\sim}{p},\underset{\sim}{r},t) = n_o(\underset{\sim}{p},\underset{\sim}{r}) + n_1(\underset{\sim}{p},\underset{\sim}{r},t) \quad , \tag{10}$$

substitute (9) into (8) and linearize:

$$\begin{aligned} &\frac{\partial}{\partial t} n_1(\underset{\sim}{p},\underset{\sim}{r},t) + \nabla_{\underset{\sim}{p}} \varepsilon(\underset{\sim}{p},\underset{\sim}{r})\cdot\nabla_{\underset{\sim}{r}} n_1(\underset{\sim}{p},\underset{\sim}{r},t) - \nabla_{\underset{\sim}{r}} \varepsilon(\underset{\sim}{p},\underset{\sim}{r})\cdot\nabla_{\underset{\sim}{p}} n_1(\underset{\sim}{p},\underset{\sim}{r},t) \\ &= \nabla_{\underset{\sim}{p}} n_o(\underset{\sim}{p},\underset{\sim}{r})\cdot\nabla_{\underset{\sim}{r}} v_1^{e}(\underset{\sim}{r},t) + \nabla_{\underset{\sim}{p}} n_o(\underset{\sim}{p},\underset{\sim}{r})\cdot\nabla_{\underset{\sim}{r}} \sum_{p'} f_{\underset{\sim}{p}\underset{\sim}{p}'}(\underset{\sim}{r})\, n_1(\underset{\sim}{p}',\underset{\sim}{r},t) \\ &- \nabla_{\underset{\sim}{r}} n_o(\underset{\sim}{p},\underset{\sim}{r})\cdot\nabla_{\underset{\sim}{p}} \sum_{p'} f_{\underset{\sim}{p}\underset{\sim}{p}'}(\underset{\sim}{r})\, n_1(\underset{\sim}{p}',\underset{\sim}{r},t) \end{aligned} \tag{11}$$

This integro-differential equation can be solved by a variety of techniques. Here we regard it as describing the flow of classical particles under the action of the Hamiltonian $\varepsilon(\underset{\sim}{p},\underset{\sim}{r})$ and with a (self-consistent) source $S_1(\underset{\sim}{p},\underset{\sim}{r},t)$ equal to the right hand side. Consequently we are led to define the following Green's function

$$\begin{aligned} G(\underset{\sim}{p},\underset{\sim}{r} \; ; \; \underset{\sim}{p}'\underset{\sim}{r}' \; ; \; t-t') = \; &\delta(\underset{\sim}{p}' - \underset{\sim}{P}(\underset{\sim}{p},\underset{\sim}{r},t')) \\ &\delta(\underset{\sim}{r}' - \underset{\sim}{Q}(\underset{\sim}{p},\underset{\sim}{r},t'))\;\; \theta(t-t') \end{aligned} \tag{12}$$

where $\underset{\sim}{Q},\underset{\sim}{P}$ describe the trajectory of a particle moving under the action of $\varepsilon(\underset{\sim}{P},\underset{\sim}{Q})$, which was created at time $\underset{\sim}{t}'$ at $\underset{\sim}{r}'$ with momentum $\underset{\sim}{p}'$ and arrives at $\underset{\sim}{r}$ with momentum $\underset{\sim}{p}$ at time t. The trajectories are given by

$$\dot{\underset{\sim}{P}} = -\nabla_{\underset{\sim}{Q}}\,\varepsilon(\underset{\sim}{P},\underset{\sim}{Q}),\quad \dot{\underset{\sim}{Q}} = \nabla_{\underset{\sim}{P}}\,\varepsilon(\underset{\sim}{P},\underset{\sim}{Q}) \tag{13a}$$

and

$$\underset{\sim}{P}(t) = \underset{\sim}{p}\ ,\quad \underset{\sim}{Q}(t) = \underset{\sim}{r} \tag{13b}$$

The formal solution of Eq. (11) is then given by

$$n_1(\underset{\sim}{p},\underset{\sim}{r},t) = \tilde{n}_1(\underset{\sim}{p},\underset{\sim}{r},t) + \int G(\underset{\sim}{p},\underset{\sim}{r};\underset{\sim}{p}',\underset{\sim}{r}';t-t')S_1(\underset{\sim}{p}',\underset{\sim}{r}',t')d\underset{\sim}{p}'d\underset{\sim}{r}'\ dt' \tag{14}$$

where $\tilde{n}_1$ is a solution of the homogeneous equation. If we now consider a single time Fourier component of v_1^e, and the corresponding density change

$$\begin{aligned} v_1^e(\underset{\sim}{r},t) &= v_1^e(\underset{\sim}{r},\omega)\ e^{i(\omega-i\eta)t} \\ n_1(\underset{\sim}{p},\underset{\sim}{r},t) &= n_1(\underset{\sim}{p},\underset{\sim}{r},\omega)\ e^{i(\omega-i\eta)t} \end{aligned} \qquad \eta = 0^+ . \tag{15}$$

then the equation (14) can be reduced to

$$n_1(\underset{\sim}{p},\underset{\sim}{r},\omega) = -\delta(\varepsilon(\underset{\sim}{p},\underset{\sim}{r}))\left[S_1(\underset{\sim}{p},\underset{\sim}{r},\omega) - i\omega\int S_1(\underset{\sim}{p}',\underset{\sim}{r}',\omega)\ G(\underset{\sim}{p},\underset{\sim}{r};\underset{\sim}{p}'\underset{\sim}{r}',\omega)\ d\underset{\sim}{p}'d\underset{\sim}{r}'\right], \tag{16}$$

where

$$S_1(\underset{\sim}{p},\underset{\sim}{r},\omega) = v_1^e(\underset{\sim}{r},\omega) + \sum_{\underset{\sim}{p}'} f_{\underset{\sim}{p}\underset{\sim}{p}'}(\underset{\sim}{r})n_1(\underset{\sim}{p}',\underset{\sim}{r}\ ,\omega) \tag{17}$$

and

$$G(\underset{\sim}{p},\underset{\sim}{r};\underset{\sim}{p}',\underset{\sim}{r}';\omega) = \int_{-\infty}^{0} ds\, e^{-i\omega s}\, \delta(\underset{\sim}{p}' - \underset{\sim}{P}(\underset{\sim}{p},\underset{\sim}{r},s))\delta(\underset{\sim}{r}' - Q(\underset{\sim}{p},\underset{\sim}{r},s)) \,. \tag{18}$$

$\tilde{n}_1$ has been omitted since, except exactly at resonance, the homogeneous transport equation has no solution.

Equation (16) is an inhomogeneous integral equation for $n_1(\underset{\sim}{p},\underset{\sim}{r},\omega)$ whose kernel G, Eq. (18), can be determined by calculating the classical trajectories, Eq. (13). From $n_1(\underset{\sim}{p},\underset{\sim}{r},\omega)$ the induced particle density is given by

$$n_1(\underset{\sim}{r},\omega) \equiv \sum_{\underset{\sim}{p}} n_1(\underset{\sim}{p},\underset{\sim}{r},\omega) \,. \tag{19}$$

To treat charged systems one merely makes the replacement

$$v_1^{e}(\underset{\sim}{r},\omega) \to v_1^{t}(\underset{\sim}{r},\omega) \equiv v_1^{e}(\underset{\sim}{r},\omega) + \int \frac{n_1(\underset{\sim}{r}',\omega)}{|\underset{\sim}{r}-\underset{\sim}{r}'|}\, d\underset{\sim}{r}' \,, \tag{20}$$

the total scalar potential.

The exact linear response function, χ, is defined by the equation

$$n_1(\underset{\sim}{r},\omega) = \int \chi(\underset{\sim}{r},\underset{\sim}{r}';\omega)\, v_1^{t}(\underset{\sim}{r}',\omega)\, d\underset{\sim}{r}' \tag{21}$$

where $n_1(\underset{\sim}{r},\omega)$ is the exact induced particle density. Consider now the following approximate expression:

$$\begin{aligned}\chi(\underset{\sim}{r},\underset{\sim}{r}';\omega) = {} & \chi^{H}(\underset{\sim}{r}-\underset{\sim}{r}';\omega;\, n_o(\underset{\sim}{r})) \\ & + \chi^{LI}(\underset{\sim}{r},\underset{\sim}{r}';\, \omega;\, [n_o(\underset{\sim}{r}")]) \\ & - \chi^{LH}(\underset{\sim}{r}-\underset{\sim}{r}';\, \omega;\, n_o(\underset{\sim}{r})) \,;\end{aligned} \tag{22}$$

here χ^H is the response function of a homogeneous system of density n_o; χ^{LH} is the same quantity calculated from Landau theory; and χ^{LI} is the response function calculated in the present extension of Landau theory to inhomogeneous systems. Provided ℓ is large enough, this expression becomes arbitrarily accurate for all external perturbations $v_1^e(\underset{\sim}{r},\omega)$ regardless of the value of ω and the characteristic wave numbers q. For, in regions (II) and (III), the last two terms cancel and χ^H becomes an accurate representation; and in the remaining region ($q < \ell^{-1}$ and $\omega < v_F\ell^{-1}$), the first and last term cancel and χ^{LI} becomes an accurate representation.

The expression (22) defines the response function as a functional of the density: χ^H is determined by n_o and theoretical approximations to it are available[5]; χ^{LH} is well known in terms of the density-dependent Landau parameters[6]; and χ^{LI} can be calculated with the same Landau parameters by our theory. Thus the expression (22) can be regarded as a dynamic response function in density functional theory.

For a non-interacting one-dimensional system, Eq. (16) can be solved and leads to the following result for χ:

$$\chi(x,x',\omega) = -\frac{1}{p_F(x)}\,\delta(x-x') + \frac{i\omega}{p_F(x)p_F(x')}\,e^{i\omega t(x,x')} \qquad (23)$$

where $t(x,x')$ is the time of transit between positions x and x'. This formula has been checked by an independent calculation using the BWK approximation. It is interesting to note that for $\omega = 0$, this χ is strictly local; for $\omega \ll v_F q$ the second term is effectively small

compared to the first but of long range; and for larger ω the second term increases and becomes effectively of shorter range.

Extensions of this theory to other forms of external perturbation are under study.

Although strictly speaking our theory applies only to systems of very slow spatial variation, it should be interesting to apply it to real systems whose density varies on an atomic scale.

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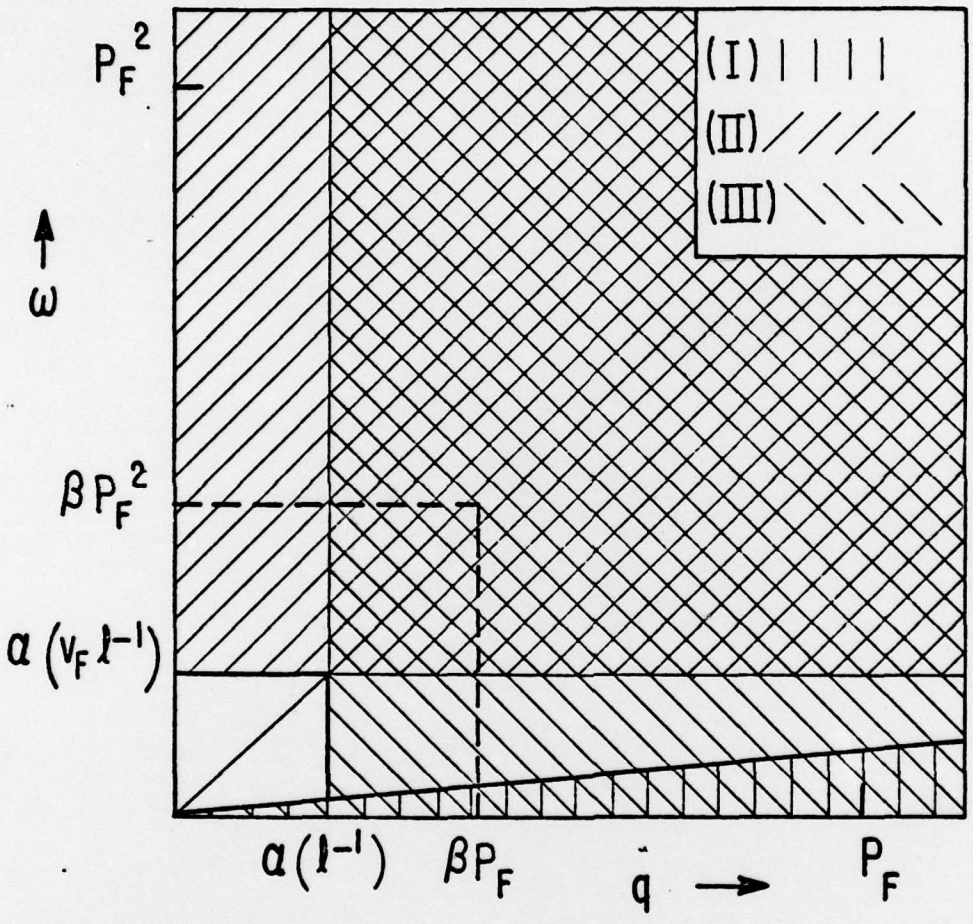
FIGURE CAPTION

Fig. 1. Region R is enclosed by heavy lines and region (IV) by the dashed lines. Local density theory is valid in regions (I), (II) and (III) but fails in region R; present theory is valid in region (IV). α is a numerical constant, large compared to unity; and β is a constant small compared to unity.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